

A condition for any realistic theory of quantum systems

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(Dated: February 1, 2008)

In quantum physics, the density operator completely describes the state. Instead, in classical physics the mean value of every physical quantity is evaluated by means of a probability distribution. We study the possibility to describe pure quantum states and events with classical probability distributions and conditional probabilities and prove that the distributions can not be quadratic functions of the quantum state. Some examples are considered. Finally, we deal with the exponential complexity problem of quantum physics and introduce the concept of classical dimension for a quantum system.

A peculiar aspect of the standard quantum formalism is interference, that is, every alternative is not associated with a probability, but with a complex number. This characteristic is at the basis of some famous paradoxes as the Schrödinger cat [1], and of the "sign problem" encountered in quantum Monte Carlo simulations [2], which gives an exponential growth of the numerical complexity. Since the birth of quantum mechanics, many physicists investigated the possibility of its description in terms of classical probabilities. Indeed, a completely equivalent alternative to the Copenhagen interpretation is Bohm mechanics [3, 4], recently extended to quantum fields with a variable particle number [5]. These approaches provide a realistic description of quantum systems. Bohm mechanics uses the same mathematical tools of the standard approach, as the wave-function, so it differs only in the interpretation and does not solve for example an important problem as the exponential complexity. The wave-function is not defined in the three-dimensional physical space, as a classical field, but in the representation space, thus the number of variables needed to define the classical state grows exponentially with the dimension of the physical system. Since quantum mechanics has a statistical interpretation, there is no a priori reason to exclude the possibility to describe the quantum states as statistical ensembles in a smaller space than the Hilbert space. In some cases, the Wigner function provides such a dimensionality reduction [7]. It has some properties of a classical probability distribution in phase-space, but in general it can take negative values. When it is positive and only particular measurements are performed, a realistic statistical description in phase-space is possible, as in the case of continuous-variable teleportation experiments involving Gaussian states and quadrature measurements [14].

In order to circumvent the sign problem of the Wigner function, some alternative non-negative probability distributions were introduced [8, 9], as the Husimi function. However, also in these cases, a realistic interpretation is not in general possible. Another example of phase-space distribution is the P-function, introduced by R. J. Glauber [10].

A realistic statistical description of quantum mechanics in a reduced phase-space is very important for its possible consequences in Monte Carlo simulations of many-

body systems. In the cases where it is possible to interpret the Wigner function as a probability distribution, as in the truncated Wigner approximation, the Monte Carlo approach allows to simulate efficiently the dynamics of atoms in degenerate bosonic gases [11] and electrons in semiconductors [12]. A general discussion of the method is also reported in Ref. [13].

In this Letter, we analyze the possibility to have a realistic description for experiments involving general states and measurements and prove that a necessary condition has to be fulfilled. Using the non-conflicting hypotheses of the theorem, we finally introduce the concept of classical dimension of a quantum system. In this Letter we use the term "classical" as equivalent to "realistic", thus, a classical theory is a theory whose variables have definite values and for which it is possible to use the classical rules of the probability theory. In this sense, Bohm mechanics is a classical theory and, consequently, every state is classical, i.e., has a realistic description.

We associate each quantum state $|\psi\rangle$ with a distribution of probability $\rho(X|\psi)$ in a suitable classical space, spanned by a set of variables X . This space can be more general than the phase-space and with higher dimensionality. No a priori hypothesis on it is introduced. We want to give physical meaning to these variables, i.e., we assume that there is an underlying theory of the quantum system described by them. When the system is prepared to a state $|\psi\rangle$, X takes a value with a probability given by ρ . If a von Neumann measurement is performed, the state collapses to a state $|\phi\rangle$ with probability $|\langle\psi|\phi\rangle|^2$. In terms of the realistic theory, we say that the system with coordinates X has a conditional probability $P(\phi|X)$ to give the event ϕ . The probability of this event, given the state $|\psi\rangle$, is obtained integrating $P(\phi|X)\rho(X|\psi)$ over X , as

$$|\langle\phi|\psi\rangle|^2 = \text{Tr}[\hat{P}_\phi \hat{P}_\psi] = \int dX P(\phi|X) \rho(X|\psi), \quad (1)$$

where $\hat{P}_\psi \equiv |\psi\rangle\langle\psi|$. The functions $\rho(X|\psi)$ and $P(\phi|X)$ have to satisfy the conditions

$$\rho(X|\psi) \geq 0 \quad (2)$$

$$\int dX \rho(X|\psi) = 1, \quad (3)$$

$$0 \leq P(\phi|X) \leq 1. \quad (4)$$

for every $|\psi\rangle$ and $|\phi\rangle$.

A relation as Eq. (1) holds when we evaluate the probability distribution of the position of a particle by means of the Wigner function. The probability to have a particle in the spatial region Ω is

$$\int dq dp P(\Omega|q, p) W(q, p) \quad (5)$$

where

$$P(\Omega|q, p) = \int_{\Omega} \delta(\bar{q} - q) d\bar{q}. \quad (6)$$

Since $0 \leq P(\Omega|q, p) \leq 1$, P it can be interpreted as a conditional probability. Thus, if the Wigner function is positive and only position measurements are involved, a realistic description in phase-space is possible [14].

Every probability distribution introduced so far is quadratic in the pure quantum state $|\psi\rangle$, as the P , the Wigner and the Q functions [10]. Indeed, the Wigner function was rigorously derived in Ref. [15] using this property and other four assumptions. We will show that quadratic distributions can not be interpreted as probability distributions of some realistic theory when general pure states and measurements are considered. More precisely, by assuming that properties (1-4) are fulfilled for *every* ψ and ϕ [16], we prove that the probability distributions associated with pure quantum states are nonlinear functions of the density operator. This is the main result of our work. Note that Bohm mechanics is a perfectly consistent realistic hidden variable theory and the corresponding probability distributions are not quadratic in the wave-function, as we will show.

In general, a positive probability distribution linear in the density operator can be obtained by means of positive operator-valued measurements (POVM) [17]. We consider a pure state $|\psi\rangle$ and define the associated probability distribution with respect to a variable X as

$$\rho(X|\psi) \equiv \text{Tr}[\hat{A}(X)\hat{P}_{\psi}], \quad (7)$$

where $\hat{P}_{\psi} \equiv |\psi\rangle\langle\psi|$ is a projector and $\hat{A}(X)$ is a generic Hermitian matrix which depends on X . X can be a vector of continuous and/or discrete variables. $\rho(X|\psi)$ must satisfy the properties (2,3). The first one is fulfilled if $\hat{A}(X)$ is positive definite, i.e. if its eigenvalues are non negative. The second one implies that [17]

$$\int dX \hat{A}(X) = \mathbb{1}. \quad (8)$$

After these preliminary remarks, we can prove the theorem. Equations (1- 4,7) are our starting hypotheses. We will show that they are conflicting.

From Eqs. (1,7), we have

$$\text{Tr} \left\{ \left[\int dX P(\phi|X) \hat{A}(X) - \hat{P}_{\phi} \right] \hat{P}_{\psi} \right\} = 0,$$

for every $|\psi\rangle$ and $|\phi\rangle$. Thus,

$$\hat{P}_{\phi} = \int dX P(\phi|X) \hat{A}(X). \quad (9)$$

Since $\hat{A}(X)$ is positive definite and $P(\phi|X) \geq 0$, it is evident that

$$P(\phi|X) \neq 0 \Rightarrow \hat{A}(X) \propto \hat{P}_{\phi}. \quad (10)$$

Thus, if $P(\phi|X) \neq 0$ and $P(\phi'|X) \neq 0$, then $\phi = \phi'$. We can define the following one-valued function

$$\chi : X \rightarrow \chi(X) \text{ such that } P(\chi(X)|X) \neq 0. \quad (11)$$

The function $\chi(X)$ spans the entire Hilbert space, but it is not necessarily invertible. It is possible to introduce an auxiliary set $Y(X)$ of variables in order to have the bijective mapping $X \leftrightarrow (\chi, Y)$. Condition (10) implies that

$$P(\phi|\chi, Y) = 0 \text{ if } \phi \neq \chi \quad (12)$$

$$\hat{A}(\chi, Y) \equiv \alpha(\chi, Y) \hat{P}_{\chi}, \quad (13)$$

where $\alpha(\chi, Y) \geq 0$. Equations (9,12,13) give

$$\int \mathcal{D}\chi dY P(\phi|\chi, Y) \alpha(\phi, Y) = 1, \quad (14)$$

for every ϕ . Since $P(\phi|\chi, Y)$ is different from zero in a set with zero measure [Eq. (12)] and it is smaller or equal to 1, $\int dY \alpha(\phi, Y)$ must be infinite for every ϕ , but this is impossible, because of the normalization condition (8). \square

Since the properties (2-4) are the minimal necessary conditions for a realistic theory, we have to discard the linear assumption, i.e., Eq. (7). This is sufficient to remove the contradiction, as shown below, when we will explicitly write the probability density and conditional probability for the Bohm theory.

Now, we consider some examples to illustrate our result. The P , Wigner and Q functions can be defined for systems described by boson creation and annihilation operators, \hat{a}^{\dagger} and \hat{a} , respectively [10]. It well-known that the P and Wigner function cannot be probability distributions. The first one is highly singular for particular states, as squeezed states or superposition of coherent states. The second one is well-defined for every state, but can assume negative values, i.e. equation (2) is not satisfied. The Q -function requires a more detailed discussion. It is smooth, positive and normalized, thus our theorem says that equation (4) cannot be satisfied. Consider a one-mode system and denote the Q -function corresponding to a state $|\psi\rangle$ by $Q(\alpha|\psi)$, where α is a complex number. The expectation value of an observable $M(\hat{a}^{\dagger}, \hat{a})$ in anti-normal form is given by the average of the function $M(\alpha^*, \alpha)$ with respect to $Q(\alpha|\psi)$. The expectation value of the number of particles

is $\langle \hat{a}^\dagger \hat{a} \rangle = \langle \hat{a} \hat{a}^\dagger \rangle - 1 = \int d^2\alpha (|\alpha|^2 - 1) Q(\alpha|\psi)$, thus we have that $\sum_{n=0}^{\infty} n P(n|\alpha) = |\alpha|^2 - 1$, where $P(n|\alpha)$ is the conditional probability of measuring n particles for the phase space state α . This equation implies that the conditional probability has to be negative for some values of n and $|\alpha|^2 < 1$, in agreement with our theorem.

Now, we consider the case of a two dimensional Hilbert space. It is possible to construct a probability distribution $\rho(n|\psi)$ with the following 3 matrices [18]: $\hat{A}_1 = \frac{1}{3}(\mathbb{1} + \hat{\sigma}_3)$, $\hat{A}_2 = \frac{1}{3}\mathbb{1} - \frac{1}{6}\hat{\sigma}_3 + \frac{\sqrt{3}}{6}\hat{\sigma}_1$ and $\hat{A}_3 = \frac{1}{3}\mathbb{1} - \frac{1}{6}\hat{\sigma}_3 - \frac{\sqrt{3}}{6}\hat{\sigma}_1$, where $\hat{\sigma}_i$ are the Pauli matrices. The distribution has three values, is positive and normalized. Also in this case, the conditional probability $P(\phi|n)$ cannot satisfy Eq. (4). For example, when $\phi = (1, 0)$, Equation (1) is fulfilled if and only if $P(\phi|1) = 3/2$ and $P(\phi|2) = P(\phi|3) = 0$.

We can define another probability distribution as $\rho(\theta, \phi|\psi) = \frac{1}{2\pi} \text{Tr}[\rho(\theta, \phi)\langle\theta, \phi|\hat{\rho}|\theta, \phi\rangle]$, where $|\theta, \phi\rangle = \cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle$ and $|0\rangle, |1\rangle$ are two orthonormal vectors. θ and ϕ are the polar coordinate of a point of the Bloch sphere. In the integrals with respect to these coordinates, we use the measure $\sin\theta d\theta d\phi$. The distribution is positive and normalized. For $|\psi\rangle = |0\rangle$, we have $\rho(\theta, \phi|0) = [\cos(\theta/2)]^2/2\pi$. The probability of obtaining the state $|0\rangle$ is equal to 1, thus

$$\int_0^{2\pi} d\phi \int_0^\pi \sin\theta P(0|\theta, \phi) \rho(\theta, \phi|0) = 1 \quad (15)$$

We assume *ab absurdo* that $P(0|\theta, \phi)$ is positive, then the equality is satisfied only if $P(0|\theta, \phi) = 1$, for $\theta \neq \pi$. But this implies that the probability to obtain $|0\rangle$ when the system is in the state $|1\rangle$ is different from zero, since the corresponding probability distribution $\rho(\theta, \phi|1) = [\sin(\theta/2)]^2/2\pi$ is zero only for $\theta = 0$. This is absurd because $|0\rangle$ and $|1\rangle$ are orthogonal. All the previous examples show that at least one property required by the theorem is not satisfied.

Discarding the linear hypothesis, we investigate how to construct a probability distribution associated with every density operator which satisfies the conditions (1-4). The Bohm mechanics provides a simple example of true probability. For sake of simplicity, here we consider only the case of a fixed number of particles [3, 4]. Recently, the theory has been extended to quantum fields and accounts for creation and annihilation of particle [5]. The dynamical variables are a multi-particle wave-function χ and the coordinates \vec{x} in the configuration space. If the quantum system is in a pure state ψ , the variable χ is merely equal to ψ and the distribution of the coordinates \vec{x} is $|\psi(\vec{x})|^2$, thus

$$\rho(\vec{x}, \chi|\psi) \equiv |\psi(\vec{x})|^2 \delta(\chi - \psi), \quad (16)$$

where ψ is the state in the Hilbert space of the quantum system. This function is obviously non-quadratic in ψ , because of the Dirac delta. In Bohm mechanics, the position measurement gives the variables \vec{x} as result,

thus, the conditional probability of finding the system in a volume Ω in the representation space is

$$P(\Omega|\vec{x}, \chi) = \int_\Omega d\vec{x}_0 \delta(\vec{x}_0 - \vec{x}). \quad (17)$$

Other measurements, for example of momentum, can be performed by a suitable unitary evolution and a subsequent measurement of position. During the evolution, the coordinates \vec{x} go to a new value which is function of x and ψ . This enables to obtain a positive conditional probability for every measurement from Eq. (17).

Bohm mechanics is a free-dispersion theory, i.e., the hidden variables fix exactly the results of measurements. It corresponds to have conditional probabilities equal to 0 or 1. This characteristic is not necessarily required by a realistic theory. Indeed, the minimal requirements are Eqs. (1-4). Discarding the free-dispersion hypothesis, the simplest probability distribution for a pure state ψ is

$$\rho(\chi|\psi) = \delta(\chi - \psi), \quad (18)$$

where χ is the variable of the classical system. The corresponding conditional probability for the event ϕ is $P(\phi|\chi) = |\langle\phi|\chi\rangle|^2$.

Although these two examples sound trivial, they show that properties (1-4) are not conflicting. At this point, we raise a question regarding the exponential complexity of quantum mechanics. In the case of Eq. (18), the dimension of the phase space spanned by the variables χ is obviously the dimension of the Hilbert space of ψ . It is well-known that the dimension of the Hilbert space grows exponentially with the physical dimension of the system. For example, it is 2^N for N spins $1/2$. Thus, also the number of variables χ of the classical theory has an exponential growth. Every known hidden variable theory has this feature. However, if we discard some required property, as positivity, the dimension of the X space can be considerably reduced. For example, the Hilbert space dimension of one boson mode is infinite, since the number of particles goes from zero to infinity, but the corresponding Wigner functions have only two variables, although we cannot regard these variables as describing a classical system, because of the negativity of the Wigner function. In general, for a Hilbert space with dimension M , it is possible to find quasi-probability distributions where X can assume only $M \times M$ values, that is, if the Hilbert space dimension is finite, we can have a space of X with dimension equal to zero. So, on one hand we have an example of true probability distribution on a space with the same dimension of the Hilbert space, on the other one, we can have quasi-probability distributions on a space with a considerably lower dimension with respect to the Hilbert space. The question we raise is the following: if the dimension of the Hilbert space is D_{quant} , which is the lowest dimension D_{class} for X in order to fulfill the conditions (1-4)? Equation (18) says that $D_{class} \leq D_{quant}$. The introduction of a probability distribution $\rho(X|\psi)$ and a conditional probability $P(\phi|X)$ for each event allows to place the question of

the exponential complexity nature of quantum mechanics onto a clear and well-defined ground and the proof that $D_{class} = D_{quant}$ or that $D_{class} \ll D_{quant}$ would cast new light upon this question. The evaluation of D_{class} is not a trivial problem and there is no evident reason for assuming it equal to D_{quant} . We have demonstrated that the solution of the problem requires to discard probability distributions quadratic in the wave-function. Note that we have not dealt with dynamical considerations, but only with the problem of a classical representation of quantum states.

In conclusion, we have studied the possibility of a classical description of quantum states and events by means of probability distributions and conditional probabilities, that must satisfy the properties (1-4). We have demonstrated that the probability distribution for a pure state has to be a nonlinear function of the density operator. We have illustrated the proof with some examples, as the P , Wigner and Q functions, and two cases of POVM for a two-state system. We have shown that for Bohm me-

chanics the distributions of probability are not quadratic functions of the pure quantum state, as required by our theorem to any realistic theory. Finally, the concept of classical dimension D_{class} of a quantum system has been introduced. Every known hidden variable theory has not a phase-space dimension smaller than the Hilbert space dimension D_{quant} . We conclude with a non-trivial question. Does a classical theory exist whose phase space dimension is much smaller than D_{quant} ? that is, is $D_{class} \ll D_{quant}$? Bohm mechanics could be considered as a pure interpretation curiosity, since it uses essentially the same tools of quantum mechanics, whereas a theory with much lower dimensionality would have important implications. We have put this problem onto a well-defined ground and its solution could clarify the nature of the exponential complexity of quantum mechanics.

I thank F. T. Arecchi for helpful discussions. This work was supported by Cassa di Risparmio di Firenze under the project "dinamiche cerebrali caotiche".

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